Multibillion-Atom Molecular Dynamics Simulations of Shockwave Phenomena on BlueGene/L

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The IBM BlueGene/L (BG/L) supercomputer at Lawrence Livermore National Laboratory consists of 65,536 nodes, each with two IBM PowerPC 440 processors (at 700 MHz clock speeds) and 512 MB of memory [1, 2] with a theoretical peak performance of 360 Tflop/s. With its three independent internal networks on BG/L, message passing times are excellent compared to most other machines.

We have ported our large-scale molecular dynamics (MD) code SPaSM [3] to the BG/L architecture and run up to 320 billion atoms to test the linear scaling of our algorithm for an enormous number of particles [4] that have never been simulated before [5]. In addition we developed a parallel graphics capability that allows for the rendering of spheres, bonds, and cells [5]. This was necessary since efficient parallel on-the-fly rendering for millions to billions of objects is not available. Here, we report on how these large-scale atomistic simulations can be applied to material science of shock wave phenomena. This work has been accepted together with two other finalists for the Gordon Bell prize performance award at the Supercomputing 2005 conference in Seattle [4].

For large-scale simulations, one would thus like to focus on fast processes, ideally with predictable simulation time requirements. Examples can be found in a variety of high strain-rate processes, including fracture (tensile and/or shear loading), sliding friction (shear loading, often along with compression), and the propagation of shock compression waves. In recent years, we have shown that nonequilibrium MD simulations can provide unprecedented insight into shock-induced plasticity 0 and solid-solid phase transitions 0. A typical simulation geometry used to study both the shock compression as well as release processes is shown in Fig. 1, which can be used to reliably estimate the required simulation time. One such simulation, involving a perfect crystal flyer plate and target with "only" 205 million atoms, is shown in Figs. 2 and 3, illustrating the spall process as well as the visualization capability. In this case, using a "centrosymmetry" order parameter 0 to distinguish fcc from non-fcc atoms provides a clear view of the plastic deformation and spall failure that occurs.

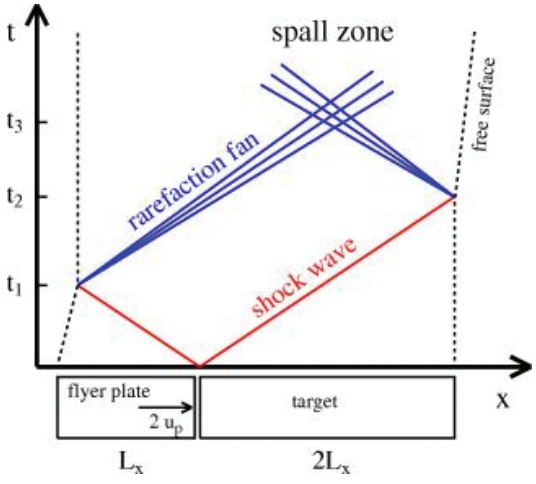

Fig. 1. ***Schematic x-t diagram showing the loading (red shock fronts) and unloading (blue expanding rarefaction fans) geometry, and relationship to required simulation times: $t1 = L_x/u_s$ is the shock transit time through the flyer plate, $t_2 = 2t_1$ the transit time through the target, and $t_3 \approx 3t_1$ the time at which the expanding rarefaction fans collide and induce a tensile region.***

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[1] N.R. Adiga, et al., "An Overview of the BlueGene/L Supercomputer," *in SC2002 – High Performance Networking and Computing*, Baltimore, MD, November 2002.
[2] G. Almasi, et al., "Unlocking the Performance of the BlueGene/L Supercomputer," *in SC2004 – High Performance Computing, Networking and Storage Conference*, Pittsburgh, PA, November 2004.
[3] D.M. Beazley and P.S. Lomdahl, *Parallel Computing* **20**, 173–195 (1994).

[4] T.C. Germann, et al., "25 Tflop/s Multibillion-Atom Molecular Dynamics Simulations and Visualization/Analysis on BlueGene/L," to appear in *Supercomputing 2005.*
[5] K. Kadau, et al., *Int. J. Modern Phys. C* **15,** 193–201 (2004).
[6] B.L. Holian and P.S. Lomdahl, *Science* **280**, 2085–2088 (1998).
[7] K. Kadau, et al., *Science* **296**, 1681–1684 (2002).
[8] C.L. Kelchner, et al., *Phys. Rev. B* **58**, 11085–11088 (1998).

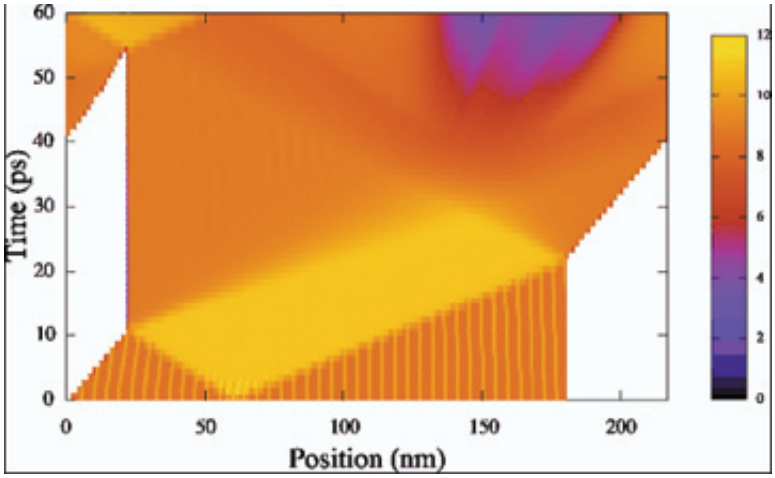

Fig. 2.
Density (in g/cc) evolution for a single crystal of copper shock-compressed in the ⟨100⟩ direction (both flyer plate and target), to particle velocity u_p = 1.0 km/s, resulting in the onset of spallation around 50 ps. The initial striations result from an incommensurability between the perfect crystal lattice and the computational bin width used to calculate densities. The target crosses the periodic boundary around 40 ps, resulting in a subsequent re-shock which is not of interest here.

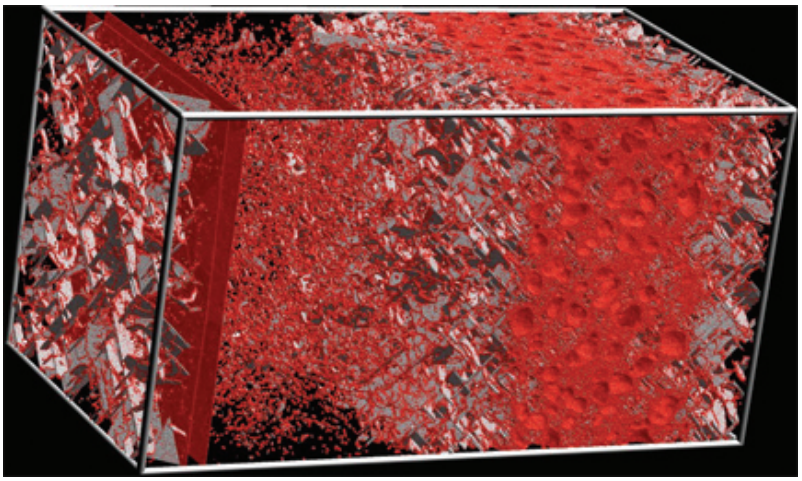

Fig. 3.
Non-fcc atoms, for the simulation shown in Fig. 2 at 50 ps. Hcp stacking fault atoms are grey, and all others red. From left to right, one can see the following features: a) stacking faults intersecting the free surface of the target, which is just about to impact the flyer plate free surface; b) residual damage (primarily in the form of point defects such as Frenkel pairs) due to shock loading and unloading in the flyer plate; and c) the nucleation of a number of voids, which will grow and coalesce to form a spall plane at later times.